**Repository Data**

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**Figure R1. GC-MS Total Ion chromatograms of various parts of *P. methysticum* stems.**

**A**, stem with peel (**SWP**), **B**,stem peel(**SP**), **C**,stem with no peel(**SNP**), and **D**, docasanoic acid in acetoneused as blank. The representative constituents identified are benzenepropanal (**b**), dihydromethysticin (**d**), hydrocinnamic acid (**h**), pipermethystine (**p**), and desmethoxyyangonin (**y**).

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**Figure R2. GC-MS Total Ion chromatograms of standards of some kava lactones found in *P. methysticum* roots.**

**A**, three kavalactones, kavain (**k**), dihydromethysticin (**d**), desmethoxyyangonin (**y**), **B**,docosanoic acid (**i**) used as internal standard.

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**Figure R3. LC-MS Total Ion chromatograms of various parts of *P. methysticum* roots** **in positive mode.**

**A**, peel of crown roots (**CRP**), **B**,crown root with no peel (**CNP**), **C**,crown root with peel (**CWP**), and **D**,lateral roots(**LR**).

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**Figure R4. LC-MS Total Ion chromatograms of various parts of *P. methysticum* stems in positive mode.**

**A**, stem with peel (**SWP**), **B**,stem peel(**SP**), **C**,stem with no peel(**SNP**), and **D,** blank

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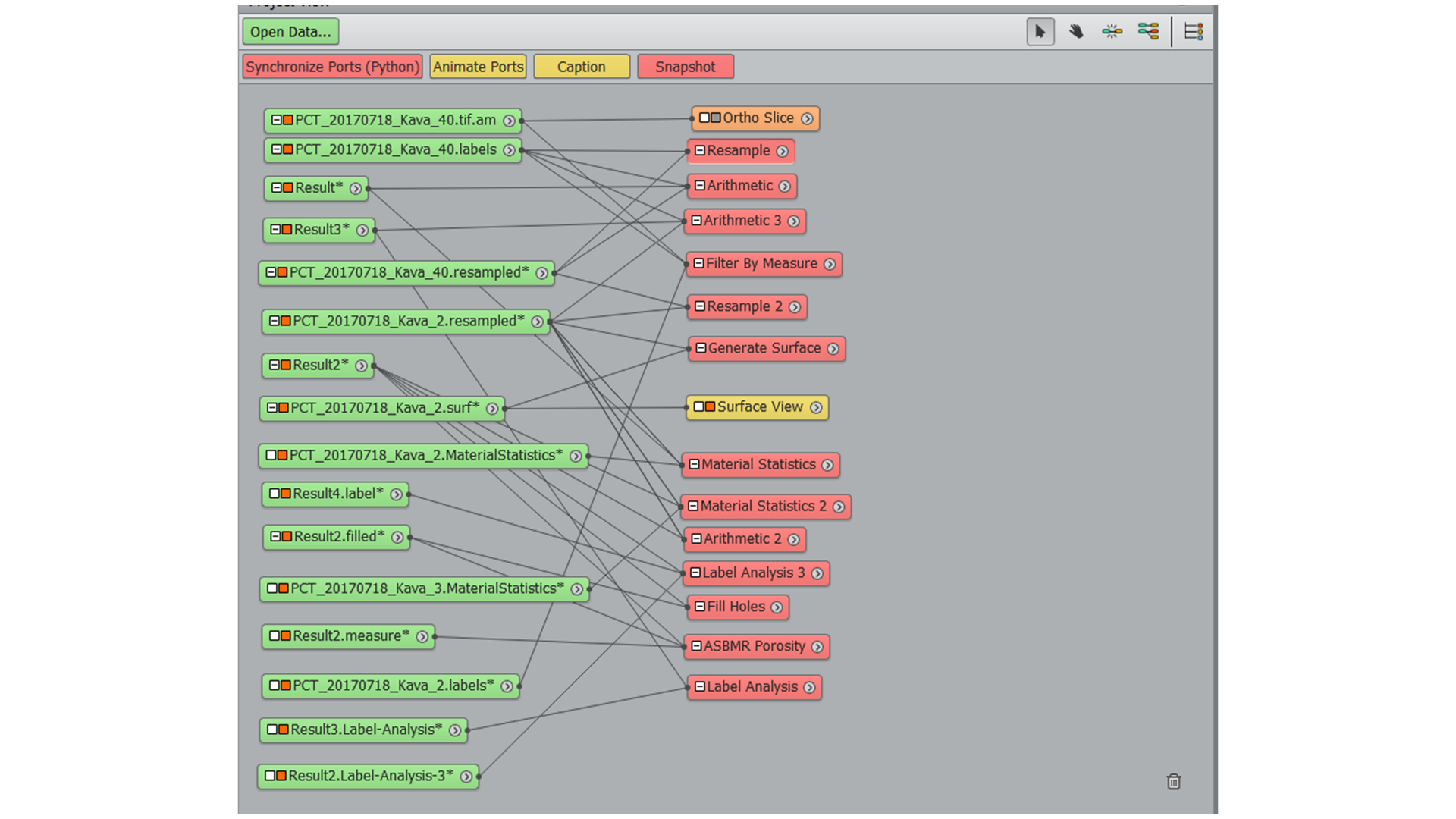
**Figure R5. LC-MS Total Ion chromatograms of various parts of *P. methysticum* roots** **in negative mode. A**, peel of crown roots (**CRP**), **B**,crown root with no peel (**CNP**), **C**,crown root with peel (**CWP**) and **D**,lateral roots(**LR**)

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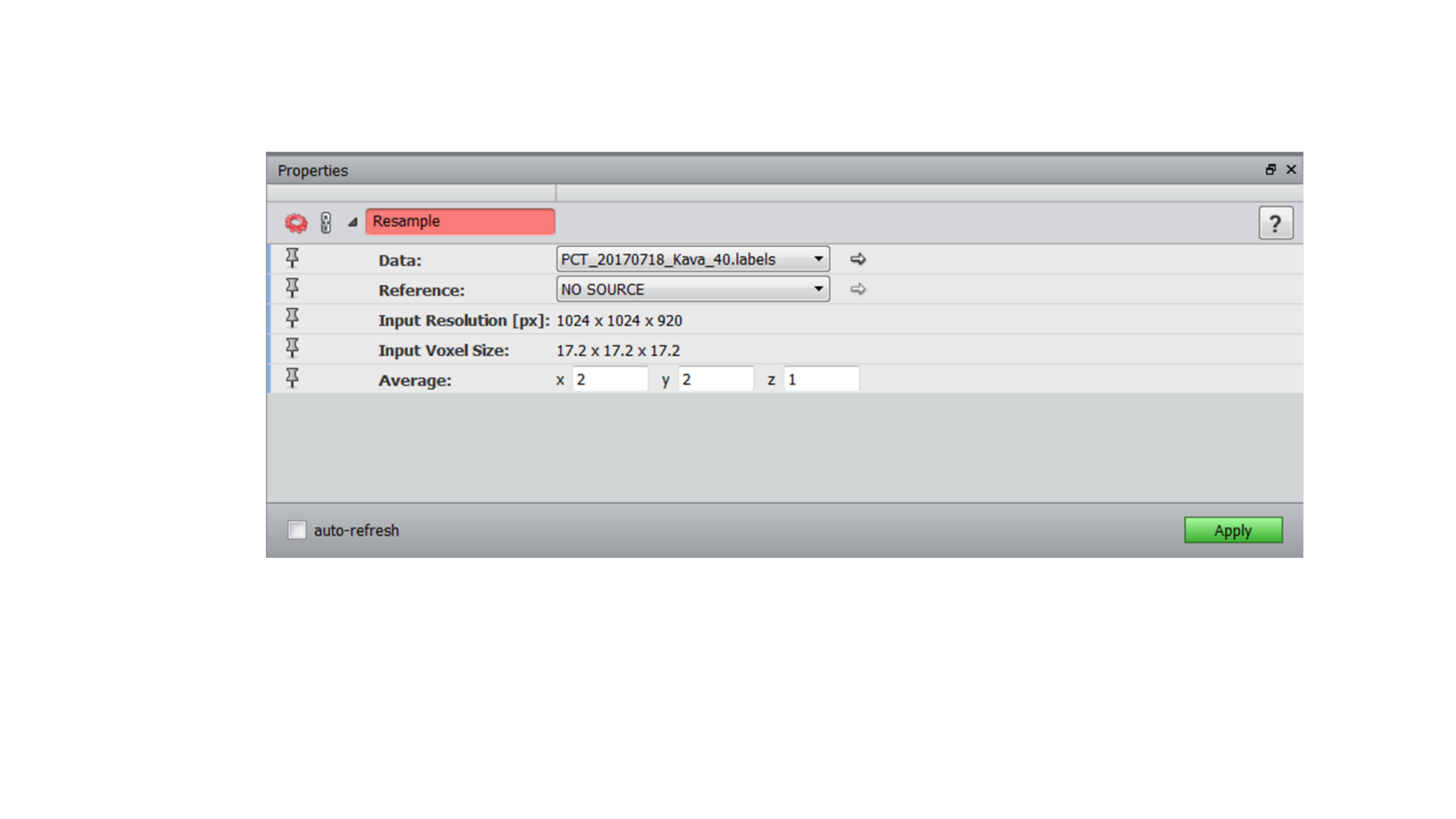
**Figure R6. LC-MS Total Ion chromatograms of various parts of *P. methysticum* stems.**

**A**, stem with peel (**SWP**), **B**,stem peel(**SP**), **C**,stem with no peel(**SNP**), and **D,** blankin negative mode.

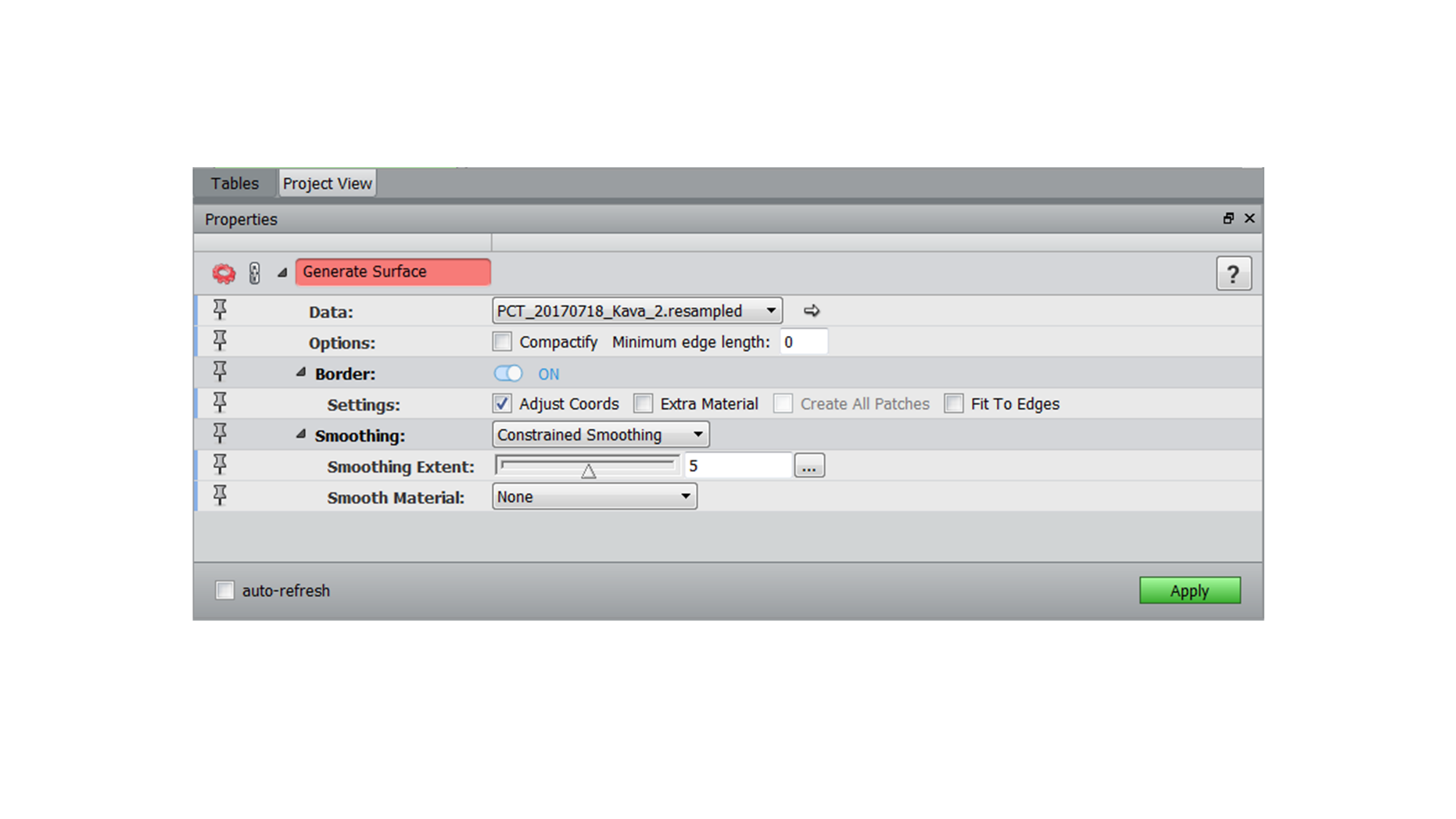
**Figure R7: Flowchart and settings for image processing, rendering and segmentation of μ-CT data with Avizo software**



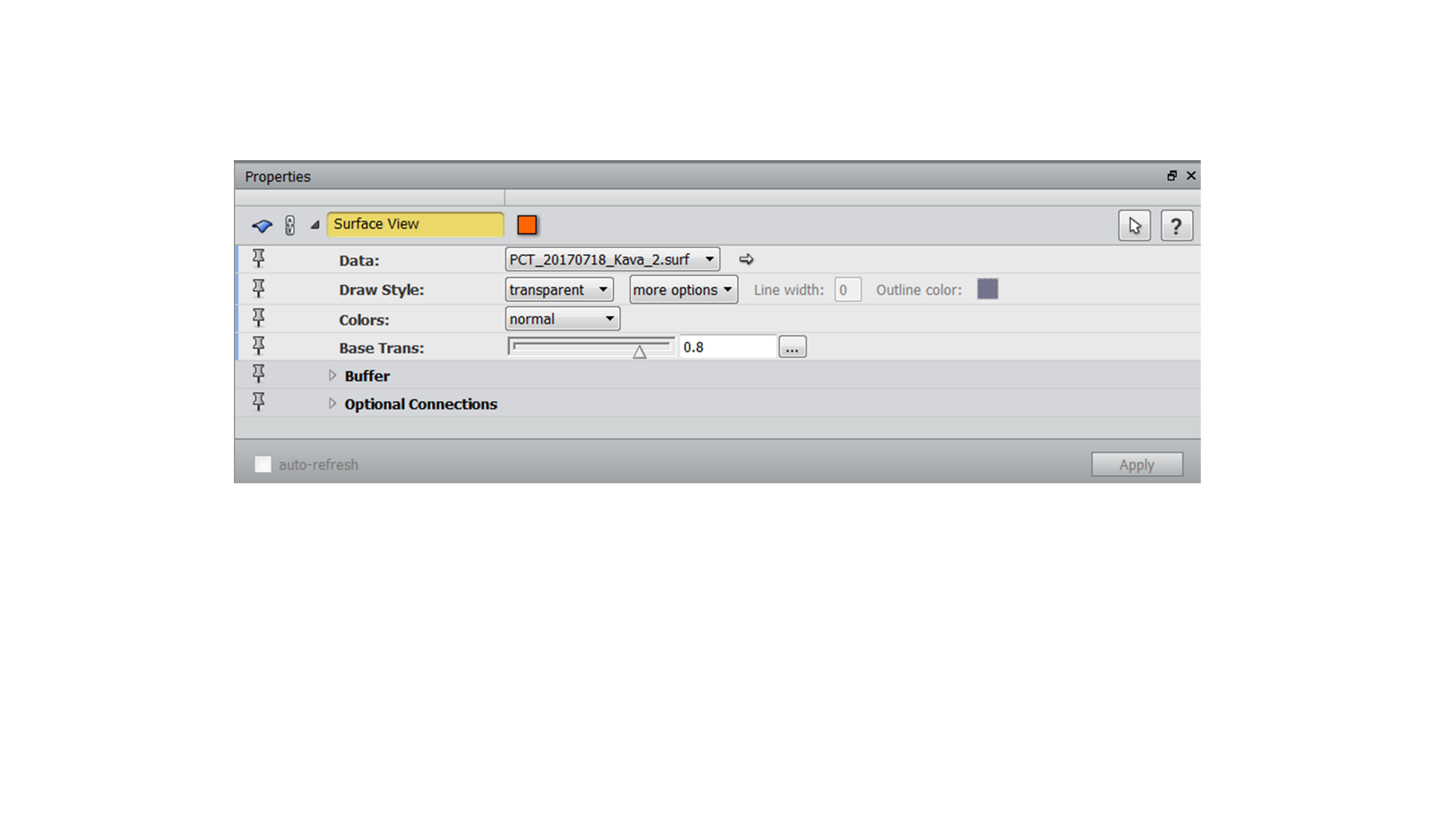
**Figure R7.1** Screenshot of 3D rendering and surface generation protocol, used for crown and lateral roots of *P. methysticum*.



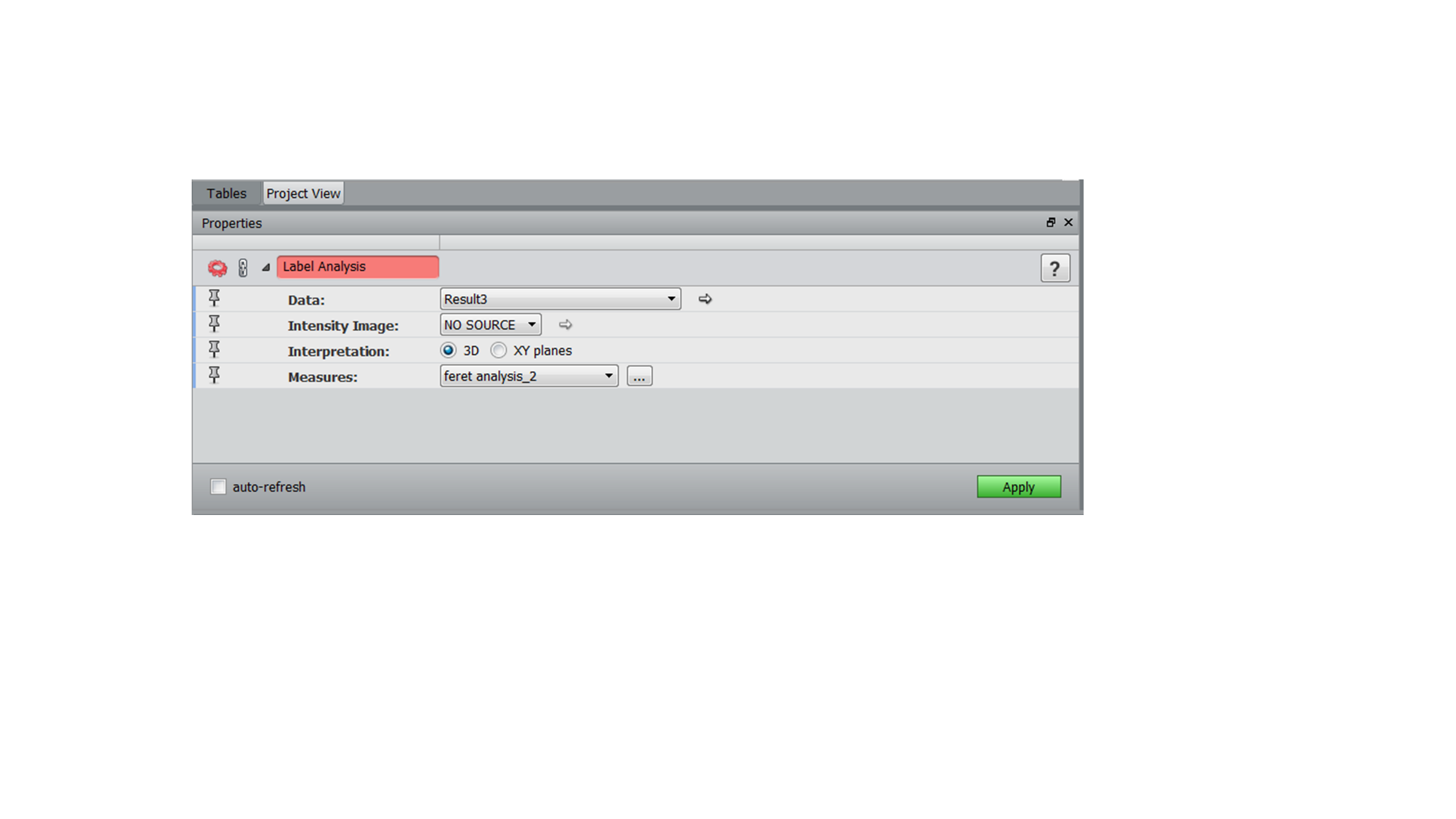
**Figure R7.2** Screenshot of ‘Resample’ module and its properties used prior to surface generation



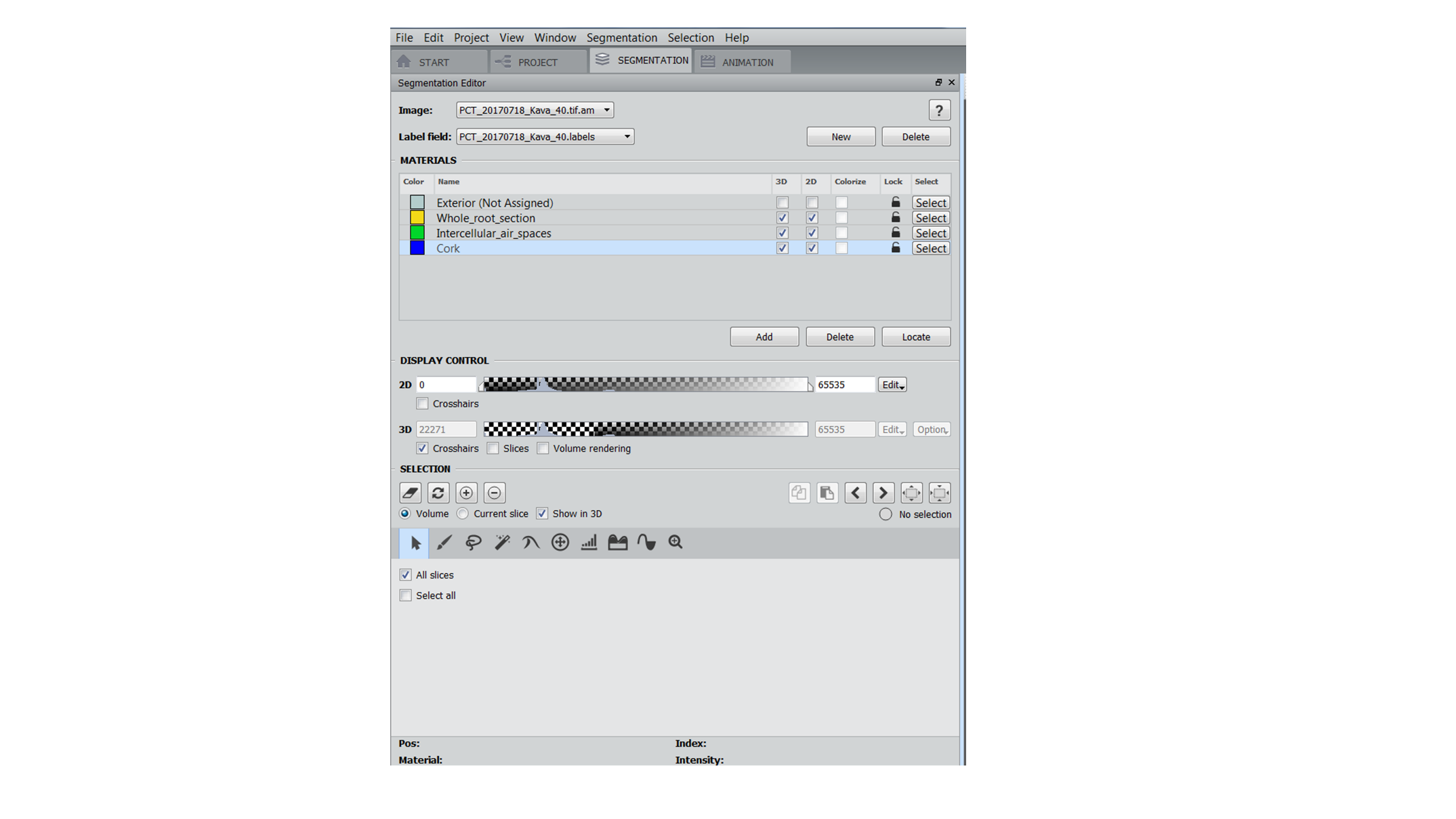
**Figure R7.3** Screenshot of ‘Generate Surface’ module and its properties



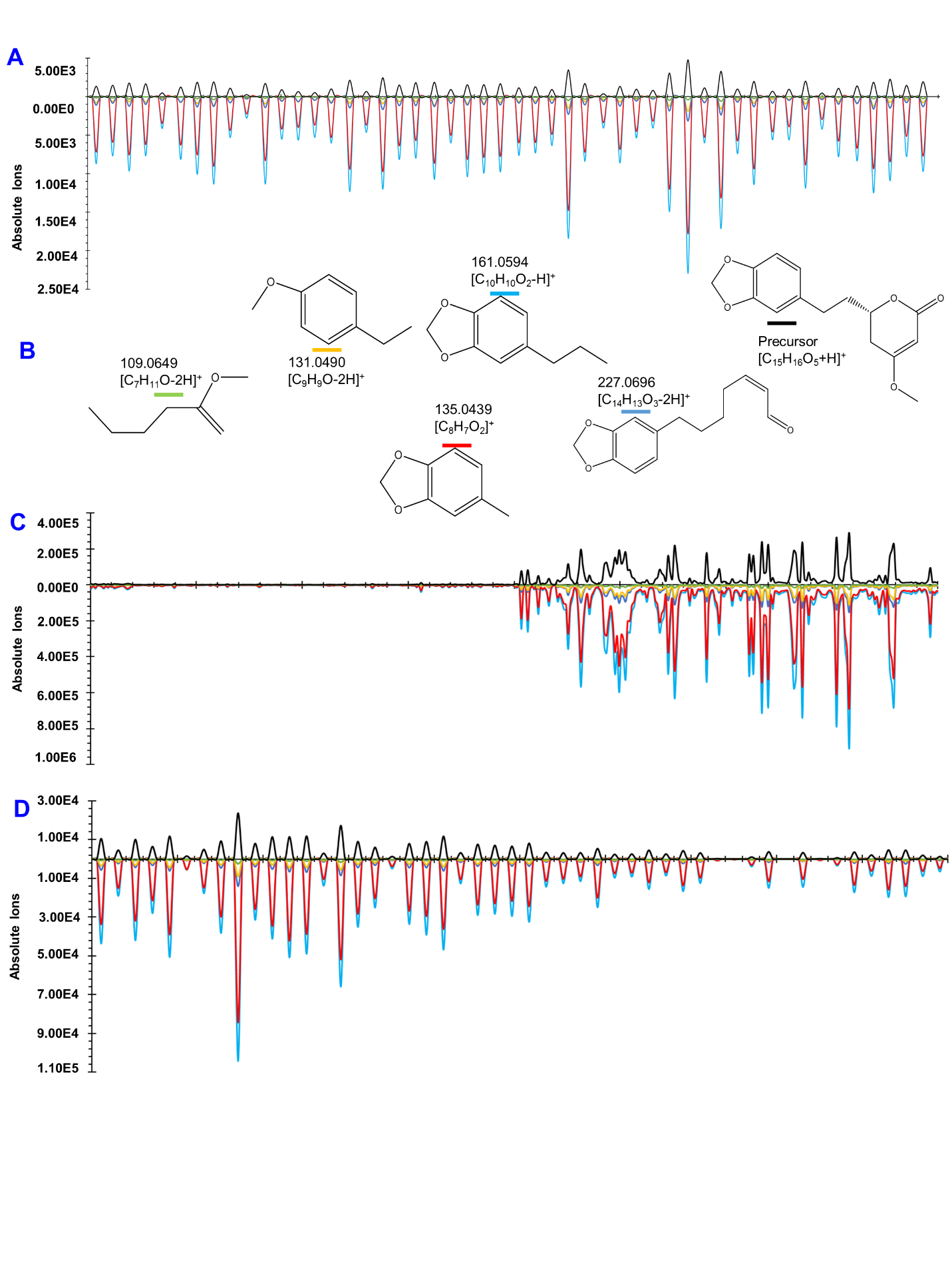
**Figure R7.4** Screenshot of ‘Surface View’ module and its properties



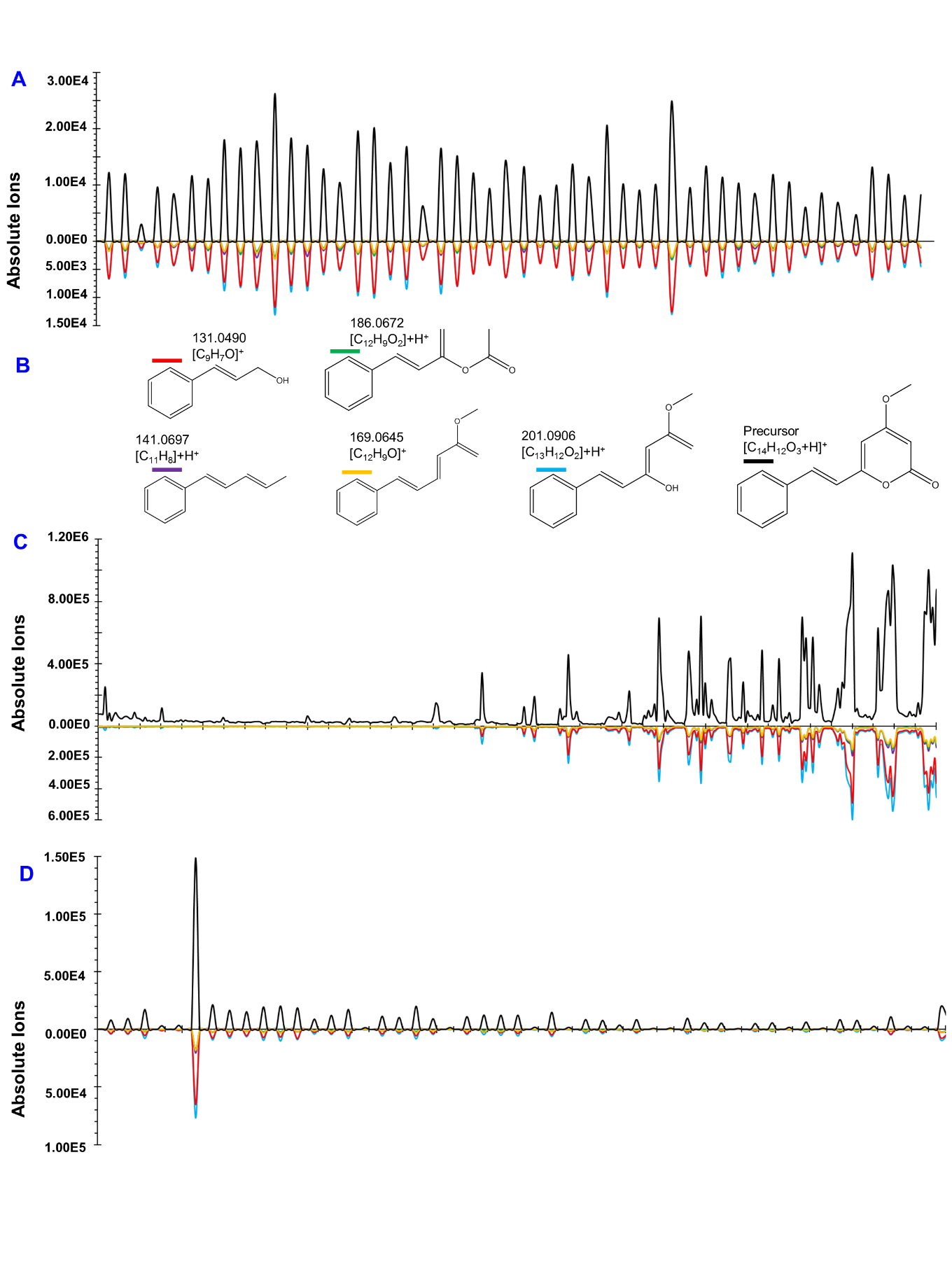
**Figure R7.5** Screenshot of ‘Label analysis’ module and its properties



**Figure R7.6** Screenshot of ‘Segmentation Editor’ and its various functions



**Figure R8. MS-MS overlay spectra and fragmentation pattern of dihydromethysticin obtained in Parallel Reaction Monitoring (PRM) MALDESI mode. (A)** represent the MS-MS spectra of standard compound, **B** represents the fragmentation pattern of dihydromethysticin, **C** and **D** represent the MS-MS spectra of kavain on crown root and stem tissues, respectively.

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**Figure R9. MS-MS overlay spectra and fragmentation pattern of desmethoxyyangonin obtained in Parallel Reaction Monitoring (PRM) MALDESI mode. (A)** represent the MS-MS spectra of standard compound, **B** represents the fragmentation pattern of dihydromethysticin, **C** and **D** represent the MS-MS spectra of kavain on crown root and stem tissues, respectively.

**File R10. Statistical analysis data files – provided as a folder in the repository:** https://github.com/palomnyk/kava\_3D\_imaging\_and\_metabolomics